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Investigation on the applicability for reaction rates adjustment of the optimized biodiesel skeletal mechanism

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ABSTRACT

In order to reduce the blindness in developing a new skeletal mechanism, a chaos genetic algorithm (CGA) is proposed for optimizing the progress of reaction rates adjustment against traditional manual operator. By this way, an optimized mechanism has been generated from a skeletal mechanism including 112 species and 498 reactions, which was reduced from a detailed mechanism consisting of 3299 species and 10806 reactions. CGA is composed by important reactions determination, fitness function building, and chaos genetic compilation. To test the applicability of the optimized biodiesel skeletal mechanism, it has been validated by 0-D ignition delay prediction and 3-D engine simulation and experiment data. Results indicate that the ignition delay error of the optimized mechanism is smaller than the skeletal mechanism by comparing with the detailed mechanism. The optimized mechanism can simulate MD and MD9D ignition behavior over a wide range of common conditions. The 3-D engine prediction results also indicated that the optimized mechanism can better present the in-cylinder combustion characteristics.

1. Introduction

It is well known that automobiles powered by internal combustion engines not only consume a lot of petroleum resources [1,2] that have become increasingly scarce, but also lead to environmental pollution [3–5]. Therefore, the development of alternative fuels as well as finding clean and efficient technology is an urgent need [6].

Biodiesel fuel is attracting increasing attention as an alternative fuel due to its inherit advantages like lower hydrocarbon and carbon monoxide emissions, renewable, carbon neutral, abundant feedstock [7–9]. So an extensive investigation on biodiesel combustion is very important [10–12]. Generally, biodiesel combustion consists of a large set of chemical processes, and the detailed mechanism maybe include thousands of species and reactions [13–17], so a detailed mechanism can't be used for CFD (Computational Fluid Dynamics) simulation directly due to lengthy computational time [18,19].

Several algorithms for detailed mechanisms reduction have been developed. For instance, Niemeyer et al. [20] developed a novel implementation DRGEPSA (directed relation graph with error propagation and sensitivity analysis) by integrating two previously developed methods DRGASA (directed relation graph-aided sensitivity analysis) and DRGEP (directed relation graph with error propagation), then compared three methods with each other. Sun et al. [21] developed a direct path flux analysis method to analyze formation and consumption fluxes of species and identify the important reaction pathways and associated species, the method have been validated by ignition delay time, PSR (Perfectly Stirred Reactor) temperature, and steady and unsteady flame propagation data. Valorani et al. [22] developed a computational singular perturbation algorithm (CSP) to generate skeletal mechanisms by eliminating unimportant reactions based on a specified error limit. Chemical isomer lumping approach [23,24] was used to lump isomer groups together and then modify the relational Arrhenius

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coefficients. Zheng et al. [25] used sensitivity analysis to find out unimportant species for removing from mechanism one by one. Zhang et al. [26] developed quasi steady state approximation (QSSA) mechanism reduction approach by combining global reduction and dynamic reduction methods.

However, the additional or removal of any species and reactions will result in some uncertain variation for mechanisms and affect the change of chemical reaction rates [27–29]. Therefore, reaction rate adjustment was conducted to compensate the changed reaction pathways for minimizing the variation and improving the ignition time predictions without changing the size of mechanism again. Generally speaking, all reaction rate coefficients should be modified [30], but most researches prefer to modify Arrhenius coefficients more [31–33]. This is due to the Arrhenius coefficient just have intuitive effects on the reaction process, but the modification of other coefficients may cause some reactions not to process.

It can be seen from aforementioned methods, reaction rates adjustment is presented as a key step in the process of mechanism reduction, but the step is absolutely depended on the repeatedly manual operator. Therefore, the Arrhenius coefficients adjustment time are unknown, because it's decided by one's experience and fate.

Among many algorithms, genetic algorithm (GA), which was developed from biological mechanism of natural selection and evolution, has become a very common tool for optimization and smart investigation [34–36]. Therefore, in order to avoid the blindness of manual operator and get the optimal results, chaos genetic algorithm (CGA) is proposed in this work. A tri-component biodiesel skeletal mechanism [32] (methyl decanoate, methyl-9-decanoate, n-heptane), as a previous mechanism, which consists of 112species and 498 reactions and was reduced from an updated mechanism consists of 3299 species and 10806 reactions [33], has been used for testing the algorithm. The result was validated by simulation and experiment data, and appeared with better accuracy when compared to the previous mechanism. It is indicated that the present CGA methodology can be used for reaction rates adjustment in the process of mechanism reduction.

2. Optimization of biodiesel skeletal mechanism

2.1. Problem description

Ignition delay time is an important parameter in the fuel oxidation. The ignition delay time in this section is the chemical ignition delay, which is identified as the time taken for the mixture temperature to increase by 400 K from its initial temperature [37,38]. The main steps for optimizing selected skeletal mechanism are expressed as follows.

1) Using SENKIN code to produce ignition delay data (τ_s) and identify important reactions from the skeletal mechanism [39].
2) Adjusting the reaction rate coefficients of these important reactions and then calculating the ignition delay time (τ_o) by a DRGEPSA code, which was developed by Niemeyer and Sung [20,40,41]. Because the previous mechanism is a reduced mechanism, the modified factors are in a narrow range of 2^{-5} to 2^5 in this work, thus the interval [-5, 5] would be defined as the gene value range.
3) Using MATLAB to read the previous mechanism, and then modifying Arrhenius coefficients of specified reactions to generate a new generation mechanism by CGA.
4) Using CGA to give the optimal adjustment according to ignition delay time.

2.2. Chaos genetic algorithm

Fig. 1 shows the implementation process of CGA. Referring to the traditional genetic algorithm, the initial population was generated by transcoding and coupling potential solutions to chromosomes according to the faced problem, each generation represents a searching space of genetic algorithm, and a fitness function about ignition delay time, which was used for calculating about each chromosome, would not be stopped until an established criteria was met. Otherwise, genetic evolution operators (selection, crossover and mutation) would be performed to generate a new better population than the previous one. Theoretically, the optimal solution consisted of several effective genes which were inherited from its parents by crossover operator, even if some effective genes lost unfortunately, mutation operator could recover these missing effective genes from chromosome. However, optimal solution losing, premature convergence and local minima maybe occur in the practice. So a chaotic variable has been complied with GA to solve the problem.

Chaos is a none-periodic, none-linear and long-term behavior. Chaos system has the randomness and ergodicity. Chaotic operator was applied to the initial population for mapping a new chaotic population as follows:

1) Establish Logistic mapping:

$$t_{i,j}(k+1) = 4t_{i,j}(k)\left[1 - t_{i,j}(k)\right] \quad (1)$$

where $i = 1, 2, \ldots, I$, represents the number of chromosomes; $j = 1,2, \ldots J$, represents the position of mutation; $k = 1,2, \ldots K$, represents

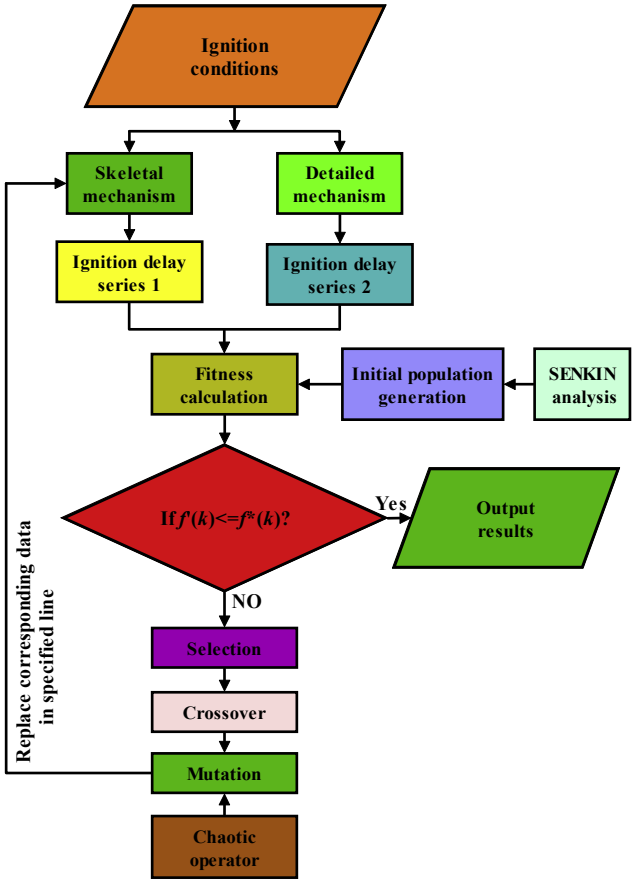

Fig. 1. CGA methodology.